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H4-alkanes: A new class of hydrogen storage material?[1] DAVID HARRISON, EVAN WELCHMAN, TIMO THONHAUSER, Wake Forest University — The methane-based material $(H_2)_4CH_4$, also called H4M for short, is in essence a methane molecule with 4 physisorbed H_2 molecules. While H4M has exceptionally high hydrogen storage densities when it forms a molecular solid, unfortunately, this solid is only stable at impractically high pressures and/or low temperatures. To overcome this limitation, we show through simulations that longer alkanes (methane is the shortest alkane) also form stable structures that still physisorb 4 H_2 molecules per carbon atom; we call those structures H4-alkanes. We further show via molecular dynamics simulations that the stability field of molecular solids formed from H4-alkanes increases remarkably with chain length compared to H4M, just as it does for regular alkanes. From our simulations of H4-alkanes with lengths 1, 4, 10, and 20, we see that e.g. for the 20-chain the stability field is doubled at higher pressures. While even longer chains show only insignificant improvements, we discuss various other options to stabilize H4-alkanes more. Our proof-of-principle results lay the groundwork to show that H4-alkanes can become viable hydrogen storage materials.

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